

Critical line of honeycomb-lattice anisotropic Ising antiferromagnets in a field

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We use numerical transfer-matrix methods, together with finite-size scaling and conformal invariance concepts, to discuss critical properties of two-dimensional honeycomb-lattice Ising spin-1/2 magnets, with couplings which are antiferromagnetic along at least one lattice axis, in a uniform external field. We focus mainly on the shape of the phase diagram in field-temperature parameter space; in order to do so, both the order and universality class of the underlying phase transition are examined. Our results indicate that, in one particular case studied, the critical line has a horizontal section (i.e. at constant field) of finite length, starting at the zero-temperature end of the phase boundary. Other than that, we find no evidence of unusual behavior, at variance with the reentrant features predicted in earlier studies.

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I. INTRODUCTION

The work reported in this paper is a study of Ising spin-1/2 systems on a honeycomb (HC) lattice, with ferro- (F) and antiferromagnetic (AF) interactions, in the presence of a uniform magnetic field. With $k = 1, 2$, and 3 being the three lattice directions, the Hamiltonian is given by:

$$\mathcal{H} = - \sum_k J_k \sum_{\langle i,j \rangle_k} \sigma_i \sigma_j - H \sum_i \sigma_i, \quad (1)$$

where the subscript $\langle i, j \rangle_k$ denotes nearest-neighbor spins along lattice direction k , and $\sigma_{i,j} = \pm 1$. Here, all fields H , coupling strengths J_k , and temperatures T will be given in units of J_1 . We only consider cases for which at least one of the J_k is negative, thus the AF character is always present.

It is well known that the two-dimensional Ising model is not amenable to exact solution when an external field is introduced. If the field is uniform and the system is AF, an ordered phase is found for suitably low values of H and T . When the zero-field ground state exhibits macroscopic entropy, the phase diagram on the $H - T$ plane shows reentrant behavior. This happens for the triangular-lattice isotropic AF [1], for which it has been found that the second-order transition along the critical line belongs to the ferromagnetic three-state Potts universality class [2–4].

If the $H = 0$ ground state has vanishing residual entropy per spin, a simpler picture is expected to hold, in which the Ising character of the zero-field transition is preserved everywhere along the critical line on the $H - T$ plane. It has been shown to be so, for isotropic AFs on both the square [5–8] and HC [8–10] lattices.

Anisotropic square-lattice Ising systems with mixed interactions (F along one lattice direction, AF along the

other) in a field have been discussed extensively; see Ref. 11 for a summary of early work, and Ref. 12 for more recent references. In this case, similarly to the pure AF the ground-state residual entropy vanishes; remarkably, reentrant behavior was found at low temperatures in some numerical or analytic treatments. While a non-trivial ground-state structure is not known to be a prerequisite for the existence of reentrances, the latter type of phenomenon usually results from subtle combinations of competing effects, whose nature it would be of importance to establish. The results of Ref. 12 indicate that the critical line starts horizontally at the zero-temperature end of the phase boundary, thus excluding reentrant behavior for this system.

For HC lattices with anisotropy, the existence of reentrances has been predicted [13] for a variety of combinations of F and AF interactions, depending also on their relative strength. In Ref. 13, an approach was used which considers the zeros of the partition function on an elementary lattice cycle, and their connection to the free energy singularity at the transition [8]. When applied to the mixed square-lattice model described in the preceding paragraph, it also predicted a reentrant critical curve [13].

Our purpose here is to establish, by numerical methods, the shape of the phase diagrams of systems described by Eq. (1), especially as regards the existence (or not) of reentrant sections; in order to do so, we necessarily probe the universality class of the phase transitions along the respective critical lines.

We use transfer-matrix (TM) methods, in connection with finite-size scaling and conformal invariance ideas, in order to produce numerically accurate phase diagrams. The underlying hypotheses in our work are: (i) that the phase transition is second-order all along the critical line, and (ii) that it belongs to the Ising universality class. Both assumptions are critically reviewed toward the end of the paper, in light of the numerical results obtained while assuming their validity.

In Sec. II we recall the calculational methods used for

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the approximate location of the critical line. In Sec. III the respective results are exhibited. In Sec. IV, we analyze the data generated in Sec. III, both in comparison with the existing literature, and in regard to their internal consistency; finally, concluding remarks are made.

II. CALCULATIONAL METHOD

A. Introduction

Referring to Eq. (1), here we consider combinations of interaction signs in which either one, two or all three of the J_k are AF. The respective strengths will be specified below in each case, in order to reproduce points in $\{J_k\}$ parameter space for which Ref. 13 predicts sizable reentrant sections of the respective critical line. As explained in the following, it is possible to do so while always keeping the couplings along two directions with the same sign and strength, while bonds along the third direction (to be denoted as *inhomogeneous*) differ from the other two in strength and/or sign.

We set up the TM on strips of width N sites, with periodic boundary conditions across. Here we use two distinct choices of orientation, respective to the lattice axes: in (a) the TM proceeds perpendicularly to one lattice direction [14], while in (b) it goes parallel to one lattice direction [10]. For (a), periodicity across the strip imposes that N must be even; no parity restrictions arise for (b). We kept to the range $4 \leq N \leq 20$, which (together with suitable extrapolation techniques) generally proved enough to yield accurate estimates of the critical lines. For the present case of anisotropic systems, and bearing in mind the definition of inhomogeneous bonds introduced in the preceding paragraph, it is possible to consider the following variants:

- (a1) choice (a), with the inhomogeneous bond perpendicular to the TM's direction of advance;
- (a2) (a), with the inhomogeneous bond along either of the remaining two directions;
- (b1) choice (b), with the inhomogeneous bond parallel to the TM's direction of advance;
- (b2) (b), with the inhomogeneous bond along either of the remaining two directions.

As these are weakly anisotropic systems [15, 16], one would expect estimates of, e.g., critical exponents and locations of critical points, to converge to the same orientation-independent limit for $N \gg 1$, while finite-size corrections should differ in each case. However, the essentially one-dimensional character of the strips used in our calculations, coupled with the distinct nature of spin couplings along the lattice axes, may introduce subtle biases when one iterates the TM along a direction which is fixed with respect to those axes. Thus, it is important to consider alternatives which at least partially compensate for such possible distortions. We used two distinct procedures, presented respectively in Sections IIB and IIC,

of which the latter is expected to be less prone to the aforementioned biases than the former.

B. Keeping $\eta = 1/4$

Following earlier work on similar problems [5, 7, 10, 12], our finite- N estimates for the critical line are found by requiring that the amplitude-exponent relation of conformal invariance on strips [17] be satisfied, with the Ising decay-of-correlations exponent $\eta = 1/4$:

$$4N\kappa_N(T, H) = \zeta\pi, \quad (2)$$

where $\kappa_N(T, H) = \ln|\lambda_1/\lambda_2|$ is the inverse correlation length on a strip of width N sites, with λ_1, λ_2 being the two largest eigenvalues (in absolute value) of the TM, and ζ is a geometric factor which compensates for the fact that on the HC lattice the strip width, in lattice parameter units, is not equal to N . One has $\zeta = 2/\sqrt{3}$ for orientation (a), and $\zeta = 1/\sqrt{3}$ for (b).

C. Phenomenological Renormalization

The assumption made in Eq (2), that the phase transition belongs to the Ising universality class, can be relaxed. Instead, one can demand only that it remain of second order. From finite-size scaling, one gets the basic equation of the phenomenological renormalization group (PRG) [18] for the critical line:

$$N\kappa_N(T, H) = N'\kappa_{N'}(T, H), \quad (3)$$

where the strip widths N and N' are to be taken as close as possible for improved convergence of results against increasing N .

Note that for PRG one is always comparing correlation lengths evaluated along the same lattice direction in Eq. (3), so the likely biases mentioned above tend to cancel out, if present [12].

PRG results can also be used as a test of the internal consistency of the Ising-universality class assumption; furthermore, should additional, non-Ising, transitions be present elsewhere in parameter space, they should be detected by PRG.

III. RESULTS

A. $J_1 = J_2 < 0$; $J_3 > 0$

Analysis of zero-field ground-state configurations shows that, in this case, N must be restricted to multiples of 4 for choice (a2) above, and to even values for choice (b2).

We take $J_3 = 1$. Consequently: (i) ground-state considerations show that $H = 2$ is the zero- T critical field,

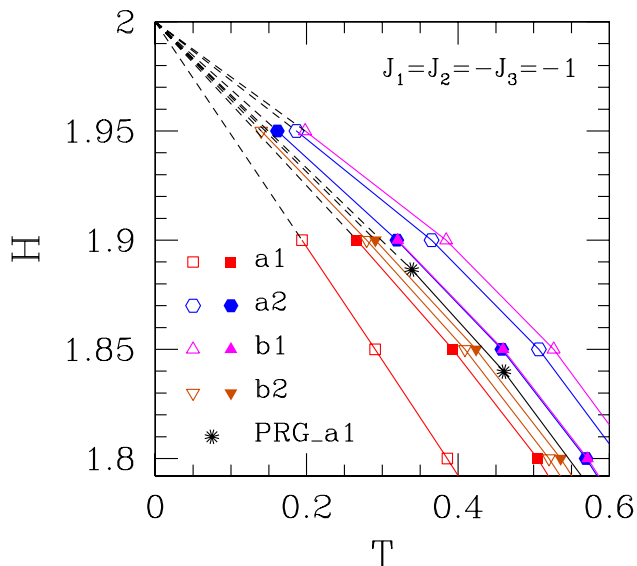


Figure 1. (Color online) For $J_1 = J_2 = -J_3 = -1$, low-temperature approximate critical boundaries given by solutions of Eq. (2) [empty symbols: $N = 4$; full symbols, $N = 14$ (a1, b1), 12 (a2, b2)], or Eq. (3) [PRG_a1: strips of widths N , $N - 2$, $N = 12$, geometry a1]. Large- N curves for a2 and b1 practically coincide on the scale shown. See text.

and (ii) the zero-field critical temperature coincides with that of the pure AF (or F) system: $T_c(H = 0) = 2/\ln(2 + \sqrt{3}) = 1.5186514 \dots$

In Ref. 13 it is predicted that, for $J_2/J_1 = |J_3/J_1| \gtrsim 0.6725$ the critical curve starts from $H = 0$ going towards higher temperatures (thus forming a "bulge") and then turns towards lower T , monotonically approaching its limiting intercept at $H = H_c(T = 0)$. Furthermore, the critical curve is predicted to reach the point $T = 0, H = H_c(T = 0)$ horizontally.

By numerically solving Eqs. (2) and (3), we found that for $H \ll 1$, the approximate critical curves leave the T axis vertically, and are very close to each other, for all possible choices (a1)–(b2) described in Section II. We find no evidence of a "bulge": $T_c(H)$ decreases monotonically with increasing H . We shall return to this point below. As H increases, differences between curves generated by the various procedures become slightly more pronounced. These are illustrated in Fig. 1. One sees that, with increasing N , all four families of solutions of Eq. (2) converge towards approximately the same intermediate location, which also coincides with the single solution of Eq. (3) shown. We have found that the solutions of Eq. (3) converge much faster with increasing N than those of Eq. (2), so the single PRG curve depicted accurately represents the $N \rightarrow \infty$ limit of its family, to the scale of the figure.

At low temperatures $T \lesssim 0.2 - 0.3$, numerical difficulties arise, because of the very large ratio between posi-

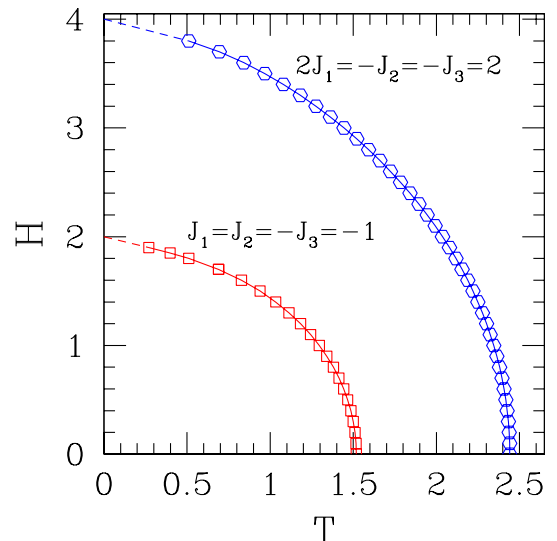


Figure 2. (Color online) Approximate phase diagrams generated by the solutions of Eq. (2), in geometry (a1) for $N=16$, for $J_1 = J_2 = -J_3 = -1$ (squares), and for $2J_1 = -J_2 = -J_3 = 2$ (hexagons).

tive and negative exponentials which are the TM states' Boltzmann weights in that region. Even accounting for this, one can see that all approximate critical curves unequivocally home in toward $(T, H) = (0, 2)$ at finite angles. This is illustrated by the dashed straight-line segments in Figure 1, which are guides to the eye only but most likely are good stand-ins for the actual shape of the corresponding curves. In conclusion, we do not find any evidence that the critical curves approach the $T = 0$ horizontally.

Going back to the predicted "bulge"-like behavior predicted at higher temperatures, Fig. 2 shows the full phase diagram generated by the solutions of Eq. (2), in geometry (a1) for $N = 16$, both for the case previously discussed of $J_1 = J_2 = -J_3 = -1$, and also for $2J_1 = -J_2 = -J_3 = 2$. This second combination has been considered because it allows direct comparison with one of the diagrams shown in Figure 12 of Ref. 13, corresponding to the same coupling values. The phase diagram obtained there exhibits a horizontal portion at $H = 4$, from $T = 0$ to $T \approx 1$, as well as a "bulge" with maximum extent at $T \approx 2.7$, $H \approx 2.3$. Here, both features are absent from the numerically evaluated critical lines.

B. $J_1 = J_2 > 0$; $J_3 < 0$

As in the case of Section III A, here N must be a multiple of 4 for choice (a2) above, and even for choice (b2).

We assume $J_3 = -1$, so (i) the zero-temperature crit-

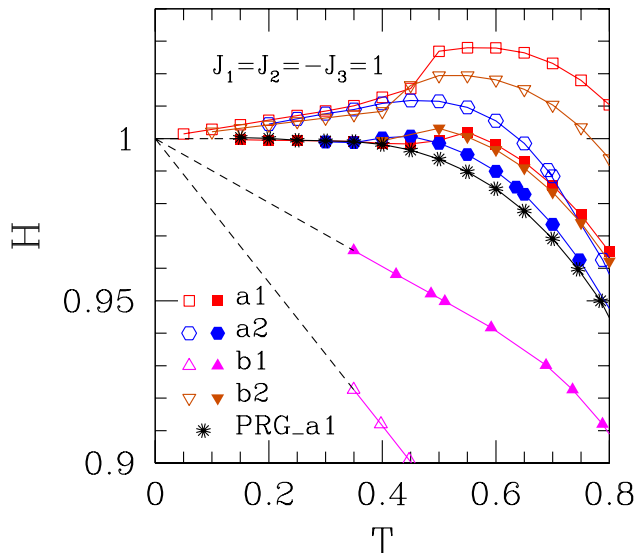


Figure 3. (Color online) For $J_1 = J_2 = -J_3 = 1$, low-temperature approximate critical boundaries given by solutions of Eq. (2) [empty symbols: $N = 4$; full symbols, $N = 14$ (a1), 16 (a2,b1), 12 (b2)], or Eq. (3) [PRG_a1: strips of widths $N, N-2, N=12$, geometry a1]. See text.

ical field is $H_c(T = 0) = 1$, and (ii) $T_c(H = 0) = 2/\ln(2 + \sqrt{3})$ as in Section III A.

In Ref. 13 it is predicted that, for $J_2/J_1 = |J_3/J_1| > 1/3$, the critical line should leave the $T = 0$ axis with positive slope. For $J_3 = -1$, from Figure 11 of Ref. 13 one sees that the peak of the corresponding reentrance is expected to occur at $T \approx 0.45$, $H \approx 1.05$. No "bulge", i.e. a section of the critical curve extending to $T > T_c(H = 0)$ at low H , is predicted.

Our results for low T , encompassing the region of the predicted reentrance, are shown in Fig. 3. For geometries (a1), (a2), and (b2), our numerical results indeed show reentrant-like behavior in the predicted range of T . However, in all three cases the evolution of the excess peak heights (i.e. above the $H = 1$ level) against increasing N is towards reduction. This is illustrated in Figure 4. It is clearly seen that the trend followed in all cases certainly excludes a positive limiting height; on the contrary, slightly negative values (≈ 0.005 in modulus) appear more likely.

The solutions of Eq. (2) in geometry (b1) do not show reentrances; their low-temperature sections approach straight lines homing in towards $(T, H) = (0, 1)$. Upon increasing N , the negative slope of such straight-line sections of the $T_c \times H$ curves becomes smaller in absolute value. A similar trend is followed by the solutions of Eq. (3) in the same geometry.

Both sets of slope values are exhibited in Figure 5. For the solutions of Eq. (2) a simple linear extrapolation of large- N data gives a negative limiting slope ≈ -0.030 .

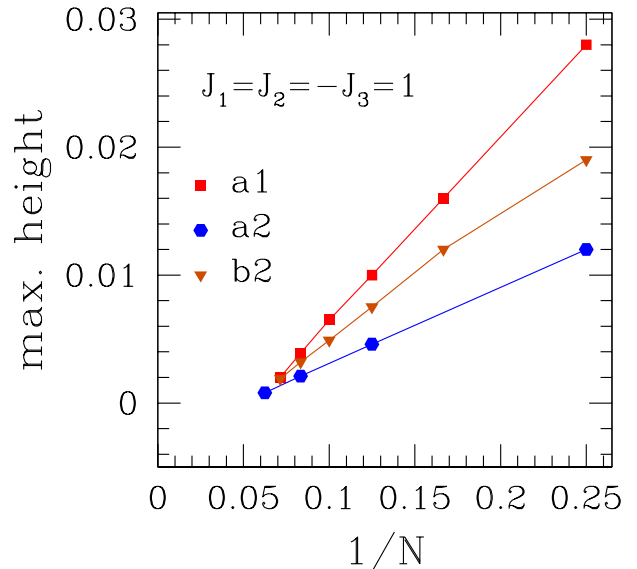


Figure 4. (Color online) For $J_1 = J_2 = -J_3 = 1$, excess peak heights (above $H = 1$) of numerically-obtained phase diagrams from solutions of Eq. (2), for geometries (a1), (a2), and (b2), against inverse strip width $1/N$. See Figure 3 for reference.

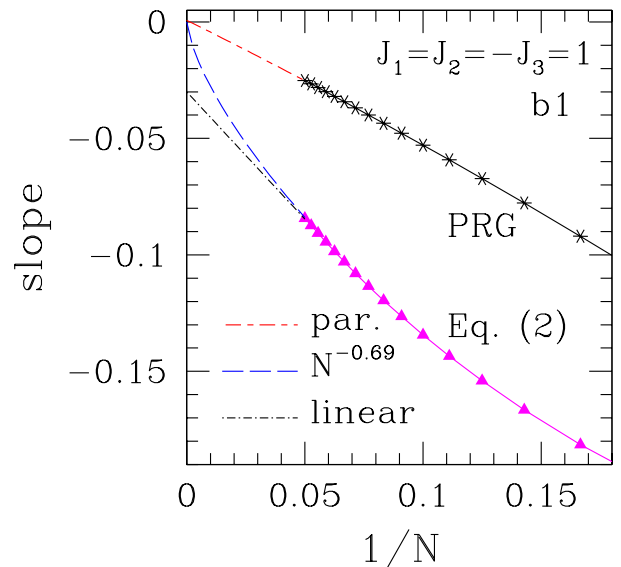


Figure 5. (Color online) For $J_1 = J_2 = -J_3 = 1$, slopes of the low-temperature straight-line sections of approximate critical boundaries given in geometry (b1), by the solutions of Eq. (2) or Eq. (3) [PRG], against inverse strip width. Data points are for $N = 6 - 20$. Lines for $N^{-1} < 0.05$ are fits of $15 \leq N \leq 20$ data to forms shown ["par." stands for "parabolic"].

Attempts to include a quadratic term (not shown) result in a limiting value around -0.015 . Fitting to a single-power form $\sim N^{-x}$, thus forcing the limiting slope to vanish as $N \rightarrow \infty$, requires $x \approx 0.69$. Though not altogether implausible, an exponent $x < 1$ means a growing amount of curvature with increasing N . Taken together, the preceding considerations indicate that a positive initial slope of the critical curve appears unlikely. The solutions of Eq.(3) in geometry (b1) behave smoothly, and a parabolic fit [i.e., with both linear and quadratic terms in $1/N$] gives a limiting slope equal to $(6 \pm 2) \times 10^{-4}$, which essentially equates to zero in the present context.

On the other hand, PRG estimates in geometry (a1) [shown in Figure 3], and also in (a2) and (b2) [not shown] consistently give the approximate critical boundary lying slightly below the $H = 1$ line (within less than 0.1% of it) for all $T \lesssim 0.4$. As remarked in Section III A, here too the solutions of Eq. (3) [other than those for geometry (b1)] exhibit very little N -dependence: for (a1), differences between results for $N = 6$ and $N = 12$ are at most of order 1–2 parts in 10^3 , with the largest values occurring midway between the phase diagram's endpoints. Thus, one cannot discard the possibility that the critical curve starts horizontally from $(T, H) = (0, 1)$, and remains flat for a finite extent, up to $T \approx 0.4$.

C. $J_1 = J_2 < 0$; $J_3 < 0$

In this case, the zero-field ground state coincides with that of the pure AF, thus there are no additional restrictions on strip widths other than those mentioned in Section II A.

We assume $J_3 = -0.4$, so (i) the zero-temperature critical field is $H_c(T = 0) = 2.4$, and (ii) $T_c^0 \equiv T_c(H = 0)$ does not take on the exact value $2/\ln(2 + \sqrt{3})$ as in Sections III A and III B.

For these coupling values, Ref. 13 predicts that the critical curve should leave the $T = 0$ axis with a positive slope, $S = \frac{3}{2} \ln 2$, see their Eq. (38) and following considerations.

The eight sets of finite- N estimates, obtained by solving Eqs. (2) and (3) in all four geometries (a1)–(b2), give very similar results, as depicted in Figure 6. In contrast with Sections III A and III B, the largest variations among differing calculational schemes are found for $H \ll 1$. At $H = 0$ we quote $T_c^0 = 1.1170(5)$, where the error bar reflects the scatter among extrapolations of finite- N sequences for each of the eight sets available. At $T = 0$ the critical curve starts with a negative slope, in disagreement with the prediction of Ref. 13.

IV. DISCUSSION AND CONCLUSIONS

For each of the three specific combinations of coupling signs and strengths discussed in Section III, we generally

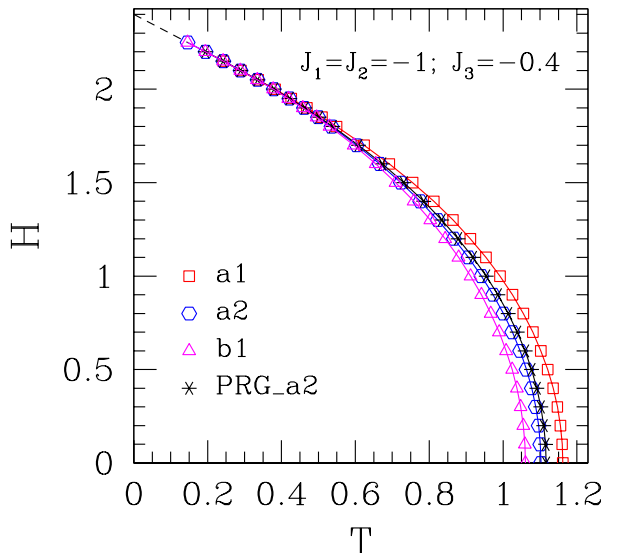


Figure 6. (Color online) For $J_1 = J_2 = -1$, $J_3 = -0.4$, examples of approximate critical boundaries from solutions of Eq. (2) (all for $N = 8$), and Eq. (3) (with $N = 10$, $N' = 8$).

found sets of solutions to Eqs. (2) and (3) in good agreement with each other, and clearly showing convergence towards the same asymptotic location of the respective phase boundaries for increasing N . We only failed to find such solutions for low temperatures, $T \lesssim 0.3$ in the worst cases. However, even in that limit we always managed to get enough data to show that the approximate critical curves are homing in towards the known zero-temperature critical field. Taken together, these considerations indicate that the phase transition between ordered and paramagnetic states remains second-order everywhere along the phase boundary [thus justifying the use of Eq. (3)], and that the transition is in the Ising universality class [which supports Eq. (2)].

With the possible exception of the low-temperature region in Section III B (to be discussed separately below), we found no evidence of reentrances, "bulges", or horizontal sections in the numerically-calculated phase diagrams here presented. Near $T = 0$ our curves leave the H axis with (negative) slope S , as defined in:

$$H_c(T) = H_c(0) + S T, \quad (4)$$

and for $H \rightarrow 0$ their shape is well fitted by a parabolic form:

$$T_c(H) = T_c(0) - a H^2. \quad (5)$$

Our estimates of S and a are given in Table I. For each set of couplings, the error bars reflect the scatter among fits of large- N approximate curves, each corresponding to one the eight possible combinations of calculational procedure and geometry. The comparison of calculated

Table I. Adjusted values of initial slope S at $T = 0$ [followed by predictions from Ref. 13], and quadratic term a in parabolic fit at $H = 0$, for phase diagrams in Sections III A–III C [see, respectively, Eqs. (4) and (5)].

Section	S	$S(\text{Ref. 13})$	a
III A	$-0.321(7)$	0	$0.205(3)$
III B	$\in [-0.03, +6 \times 10^{-4}]$	$(1/4) \ln 2$	$0.504(2)$
III C	$-0.995(5)$	$(3/2) \ln 2$	$0.158(1)$

initial slopes with the predictions of Ref. 8, summarized in Table I, bears strong resemblance to the discussion of Ref. 12 for similar systems on a square lattice. Also, as remarked there, it is worth recalling the comparable problem of isotropic antiferromagnets (on both square and HC lattices): although the critical lines $H_c(T)$ given in Ref. 8 do not exhibit reentrances, they are always above those found in Refs. 6 and 7 (except at the $T = 0$ and $H = 0$ ends, where the lines coincide in both cases). Thus the results presented here are consistent with previous ones, in indicating that the methods employed in Refs. 8 and 13 tend to overestimate the extent of the ordered region in parameter space.

Going back to the low-temperature region of the phase diagram in Section III A, the behavior seen there strongly suggests that the critical line approaches the $T = 0$ axis at a very low angle, possibly even horizontally or (though less likely) at a very slight reentrance. The range of slope estimates given in Table I reflects the arguments given

in connection with Figures 3, 4, and 5. Similar behavior occurs in the square-lattice metamagnet studied in Ref. 12, where a sizable extent of the low-temperature phase boundary is found to be horizontal to within 0.1% (the same fractional deviation exhibited by the PRG curves here, see Section III B).

In the three-dimensional version of the problem of Ref. 12, it is known that a tricritical point occurs at low temperatures [19]. As shown in Figure 3, we managed to find solutions of Eq. (3) [whose validity is based on the assumption of a second-order transition] for rather low T . Furthermore, in that region the approximate critical curves are well-behaved as far down in temperature as we can ascertain, pointing directly towards the $T = 0$ critical field. Thus no evidence has been found that the nature of the transition changes, or is about to change, close to $T = 0$.

In conclusion, we have found strong indications that reentrant behavior does not occur in the systems studied here, for which the ground state has a relatively simple structure. On the other hand, even for these systems it is possible to find slightly unusual features such as horizontal sections of the phase diagram, which it does not obviously suggest themselves.

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| <p>[1] W. Kinzel and M. Schick, Phys. Rev. B23, 3435 (1981).
 [2] Z. Rácz and T. Vicsek, Phys. Rev. B27, 2992 (1983).
 [3] J. D. Noh and D. Kim, Int. J. Mod. Phys. B 6, 2913 (1992).
 [4] S. L. A. de Queiroz, T. Paiva, J. S. de Sá Martins, and R. R. dos Santos, Phys. Rev. E59, 2772 (1999).
 [5] H. W. J. Blöte and M. P. M. den Nijs, Phys. Rev. B37, 1766 (1988).
 [6] X.-N. Wu and F. Y. Wu, Phys. Lett. A 144, 123 (1990).
 [7] H. W. J. Blöte and X.-N. Wu, J. Phys. A 23, L627 (1990).
 [8] X.-Z. Wang and J. S. Kim, Phys. Rev. Lett. 78, 413 (1997).
 [9] F. Y. Wu, X. N. Wu, and H. W. J. Blöte, Phys. Rev. Lett. 62, 2773 (1989).
 [10] H. W. J. Blöte, F. Y. Wu, and X. N. Wu, Int. J. Mod. Phys. B 4, 619 (1990).</p> | <p>[11] C. Rottman, Phys. Rev. B41, 2547 (1990).
 [12] S. L. A. de Queiroz, Phys. Rev. E80, 041125 (2009).
 [13] X.-Z. Wang and J. S. Kim, Phys. Rev. E56, 2793 (1997).
 [14] V. Privman and M. E. Fisher, Phys. Rev. B30, 322 (1984).
 [15] P. Nightingale and H. Blöte, J. Phys. A 16, L657 (1983).
 [16] A. Hucht, J. Phys. A 35, L481 (2002).
 [17] J. L. Cardy, in <i>Phase Transitions and Critical Phenomena</i>, Vol. 11 (Academic, New York, 1987), edited by C. Domb and J. L. Lebowitz.
 [18] M. P. Nightingale, in <i>Finite Size Scaling and Numerical Simulations of Statistical Systems</i>, (World Scientific, Singapore, 1990), edited by V. Privman.
 [19] F. Harbus and H. E. Stanley, Phys. Rev. Lett. 29, 58 (1972).</p> |
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